

*Scientific and Technical Report No. 12*

# River Water Quality Model No. 1

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*Edited by*

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**Published by IWA Publishing, Alliance House, 12 Caxton Street, London SW1H 0QS, UK**

Telephone: +44 (0) 20 7654 5500; Fax: +44 (0) 20 7654 5555; Email: [publications@iwap.co.uk](mailto:publications@iwap.co.uk)

Web: [www.iwapublishing.com](http://www.iwapublishing.com)

First published 2001

© 2001 IWA Publishing

Edited and typeset by Jane Hammett, Leighton Buzzard, Bedfordshire, UK.

Printed by TJ International (Ltd), Padstow, Cornwall, UK

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*British Library Cataloguing in Publication Data*

A CIP catalogue record for this book is available from the British Library

*Library of Congress Cataloging-in-Publication Data*

A catalog record for this book is available from the Library of Congress

ISBN: 1 900222 82

# Acknowledgements

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This report was prepared by the IWA Task Group on River Water Quality Modelling. László Somlyódy conceived of the Task Group and served as its chair. Peter Shanahan served as editor of this report from the Task Group.

Portions of this report have previously been published in modified form in *Water Science and Technology* by Rauch *et al.* (1998b)<sup>1</sup>, Shanahan *et al.* (1998), Somlyódy *et al.* (1998), Shanahan *et al.* (2001), Reichert *et al.* (2001a), Vanrolleghem *et al.* (2001), Reichert (2001), Borchardt and Reichert (2001), and Reichert and Vanrolleghem (2001).

The Task Group greatly appreciates the financial support of IWA and the editorial assistance of Jane Hammett.

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<sup>1</sup> Dr László Koncsos contributed as an earlier member of the Task Group.



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# 1

## Introduction

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### 1.1 BACKGROUND

River water quality modelling has a long history that dates back to the pioneering work of Streeter and Phelps in 1925. Streeter and Phelps described the bacterial decomposition of organic carbon characterised by biochemical oxygen demand (BOD) and its impact on dissolved oxygen conditions. In the course of the next half-century, this simple, first-order kinetics approach was further developed in three major steps. The first was the refinement of the two-state-variable model by introducing the settling rate (of particulate matter) in addition to the decay rate (of dissolved matter) and the so-called sediment oxygen demand (as a parameter). The model was also improved by using research results on the surface reaeration rate. Finally, an extension was made by distinguishing between carbonaceous BOD (CBOD) and nitrogenous BOD (NBOD), which led to a third state variable. The second step was the incorporation of a simplified nitrogen cycle: ammonia, nitrate, and nitrite appeared as new components. This extension appears in QUAL1 (TWDB 1971), the first model of the QUAL family. Ten years later the third step further extended the approach by incorporating phosphorus cycling and algae, which resulted in organic nitrogen, organic phosphorus, dissolved phosphorus, and algae biomass (in terms of chlorophyll *a*) as additional state variables. This model is known today as QUAL2E and is widely used. It has also been adopted in a practically unchanged form in various simulation software and decision support systems (DSS).

The above brief summary suggests a rather natural evolution. The three subsequent steps represent three different concepts (Masliev *et al.* 1995). The original Streeter–Phelps model is a phenomenological model, where BOD is not the concentration of a chemical substance, but the result of a bioassay test. The models of the second step have a typical chemical kinetic structure, where a group of first-order reactions represent in a cumulative manner the complex chain of processes related to electron transfer in aerobic conditions. Finally, in the third step, the algae model is an ecosystem dynamics model that accounts for non-linear growth and decay of phytoplankton and nutrient cycling. Since the procedure of model development was based mostly on the incorporation of “incremental” impacts by a more or less mechanical addition of model layers, these models contain inconsistencies. They also often lack clear operational definitions of the water quality variables involved.

Bacterial decomposition also takes place under well-controlled conditions in biological wastewater treatment plants. Models have been applied here for several decades, as well. However, the development history is rather different than that for rivers. In 1987 the IAWPRC<sup>1</sup> Activated Sludge Model (ASM) No. 1 was published (Henze *et al.* 1987). It was developed *in one piece* by a co-ordinated effort of professionals sharing a unified conceptual basis. The conceptual basis had developed as a standard model on the basis of experience gained with earlier activated sludge process models.

The ASM1 effort led to a useful cross-fertilisation. Some of the researchers working in the field of water quality modelling (see for example Masliev *et al.* 1995; Maryns and Bauwens 1997) raised obvious questions about the similar processes in the two sets of models. While there are differences in the order of magnitude of biomass and concentrations between natural conditions in rivers and well-controlled conditions in reactors, it is nonetheless logical to ask, to what extent are QUAL2 and ASM1 similar to each other? Can one not draw conclusions from such a comparison for future model development? Could the two models be linked to each other to handle wastewater treatment plants (WWTPs) and rivers in an integrated fashion? And finally, would it not make sense to launch a systematic model development and harmonisation effort also for river water quality models?

The implications of the above thoughts were strengthened by strategic needs in Europe. During the past few years significant efforts have been made to develop the EU–Water Framework Directive (approved October 2000; EU 2001a,b), which formed the basis of water policy for the European Union and associated countries. The basic goal of the EU-WFD is to achieve “good status” of both surface and ground waters within given time periods with a strong focus on ecological criteria and by strategic integrated management. EU-initiated management and research activities clearly focus on integrated water resources management and the development of harmonised tools supporting it. Similar needs may show up in the future in other continents and large countries, for example, Australia.

The establishment of the IWA Task Group on River Water Quality Modelling was an obvious consequence of all the above. The task group was formed to create a scientific and technical base from which to formulate standardised, consistent river water quality models and guidelines for their implementation. This effort was intended to lead to the development of river water quality models that are compatible with the existing IWA Activated Sludge Models (ASM1, ASM2 and ASM3; Henze *et al.* 2000) and can be straightforwardly linked to them. To this end, water quality components and model state variables characterising carbon, oxygen, nitrogen, and phosphorus cycling are a necessary part of the river model.

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<sup>1</sup> International Association on Water Pollution Research and Control. Later, IAWPRC was renamed to IAWQ and now IWA.

## 1.2 PROBLEM DEFINITION

Water quality models are used for many different problems and purposes. Existing models address some of these problems better than others. We have named the model presented in this report River Water Quality Model No. 1 (RWQM1). We have used a name similar to ASM1 to express the hope of initiating a similar development process as achieved for activated sludge models. Applications that RWQM1 is intended to address include:

- (1) dynamic problems of combined stormwater overflows and non-point source pollution;
- (2) impact of improved wastewater treatment plant operation and control;
- (3) extreme and surprising pollution events;
- (4) improved assessment of artificially influenced rivers (for example, by dams or re-naturalisation);
- (5) data collection;
- (6) structured understanding, research, education, and improved communication (e.g. between wastewater engineers and receiving water quality experts); and,
- (7) regulatory applications including catchment planning.

Chapter 7 provides additional discussion with respect to addressing these different types of applications.

## 1.3 CONTEXT

Water quality changes in rivers are due to physical transport processes and biological, chemical, biochemical, and physical conversion processes. Physical transport includes advection and turbulent diffusion, which are separately described through hydraulic models. The above processes in the water phase are governed by a set of extended transport equations that can be represented conceptually as:

$$\boxed{\begin{array}{c} \text{Change in} \\ \text{concentration} \\ \text{with time} \end{array}} = \boxed{\begin{array}{c} \text{Change} \\ \text{due to} \\ \text{advection} \end{array}} + \boxed{\begin{array}{c} \text{Change due to} \\ \text{diffusion or} \\ \text{dispersion} \end{array}} + \boxed{\begin{array}{c} \text{Change due to} \\ \text{conversion} \\ \text{processes} \end{array}} \quad (1.1)$$

To this conceptual equation, a similar mass conservation equation for the sediment should be added. Interface terms (e.g. sediment–water and water–air) appear as boundary conditions that are completed by specifying in- and outflows and boundary fluxes. Depending on integration, boundary conditions may enter the equation as sink or source terms (as a part of the aggregated conversion processes term).

If we compare our knowledge on advection, dispersion, and their hydraulic backgrounds on the one side and conversion processes (mostly related to chemistry and biology) on the other side, clearly we are much weaker on the latter “soft” field. Here data collection, experimentation, and general empirical knowledge play a decisive role in identifying the model or submodel structure, and in performing model calibration and validation. This is particularly the case if we consider the uncertainties inherent in field data, model structure, and parameter values. Thus, methodologically three main components of the modelling context should be distinguished: (a) advection, dispersion, and hydraulics; (b) conversion

processes; and (c) analyses related to identification, calibration, validation, and uncertainty. In this report we will deal primarily with the second element, conversion processes.

## 1.4 OBJECTIVES OF RWQM1

Our goal is to deal solely with the development of conversion submodels for traditional pollutants. This choice of focus is similar to that which led to the IWA Activated Sludge Models. Our choice recognises that there are well-developed models and tools to address the physical transport components of this problem. Particularly, one-dimensional, two-dimensional, and, increasingly, three-dimensional hydrodynamic models are available to determine the velocity field and are becoming more practical with advancements in computer technology. We therefore see the future in water quality modelling as resting on the development of a well-structured description of conversion processes in Equation (1.1).

On the basis of reviewing the state of the art and the problems with that state of the art, we define our detailed objectives as:

- (1) to develop a sequence of coherent and improved conversion submodels ranging from simple to complex;
- (2) to guide the selection of (a) hydraulic and physical transport model components, and (b) process submodels, and (c) to test the resulting water quality model; and,
- (3) to apply the submodels to real data from selected case studies.

The first of these objectives entails the following subtasks:

- to re-evaluate models developed during the past three decades and to eliminate such inherent inconsistencies as the lack of closed mass balances (which mostly arise from an inadequate description of sediment-related processes and the use of BOD for the characterisation of organic matter);
- to guarantee compatibility with the IWA Activated Sludge Models to enable integrated analysis of wastewater treatment and receiving water quality impacts;
- to include and improve process descriptions such as nitrification, denitrification, and those related to sediment, benthic fluxes, attached bacteria and algae, and macrophytes; and,
- to formulate the resulting models in a way that is based on the innovative formalism used in the activated sludge models but at the same time considers the needs and practices of biologists, chemists, and other professionals dealing with rivers.

We expect these changes in model formulation to improve the predictive power of models to estimate multiple and non-linear effects from changes in emissions and other artificial alterations.

## 1.5 METHOD OF MODEL PRESENTATION

The following discussion is excerpted almost verbatim from Henze *et al.* (1987). We have adopted the identical model presentation method as employed by Henze *et al.* for the Activated Sludge Model No. 1, both to ensure compatibility with ASM1 and to take advantage of the intrinsic attractiveness of this simple and clear method, which has not previously been employed in river water quality modelling.

Simulation of activated sludge (and river) system behaviour, incorporating phenomena such as carbon oxidation, nitrification, and denitrification, must necessarily account for a large number of reactions between a large number of components. To be mathematically tractable while providing realistic predictions, the reactions must be representative of the most important fundamental processes occurring within the system. In this context the term “process” is used to mean distinct mechanisms acting upon one or more system components. Furthermore, the model should quantify both the kinetics (rate-concentration dependence) and the stoichiometry (relationship that one component has to another in a reaction) of each process. Identification of the major processes and selection of the appropriate kinetic and stoichiometric expressions for each are the major conceptual tasks during development of a mathematical model. Consequently, most of this report will concern them.

### 1.5.1 Format and notation

One problem often associated with papers presenting models describing complex systems is that it is difficult to follow the development of the author’s ideas. In particular, it is often difficult to trace all the interactions of the system components. Henze *et al.* (1987) concluded that a matrix format, based on the work of Petersen (1965), for presentation of the model offered the best opportunity for overcoming this problem while conveying the maximum amount of information. Furthermore, they felt that the notation recommended by a previous Task Group (Grau *et al.* 1982) should be used. An illustration will introduce the matrix format and the notation.

Consider a situation in which heterotrophic bacteria are growing in an aerobic environment by utilising a soluble substrate for carbon and energy. In one simple conceptualisation of this situation, two fundamental processes occur: the biomass increases by cell growth and decreases by decay. Other events, such as oxygen utilisation and substrate removal, also occur, but these are not considered to be fundamental because they result from biomass growth and decay and are coupled to them through the system stoichiometry. The simplest model of this situation must consider the concentrations of three components: biomass, substrate, and dissolved oxygen. The matrix incorporating the fate of these three components in the two fundamental processes is shown in Table 1.1.

Table 1.1: Process kinetics and stoichiometry for heterotrophic bacterial growth in an aerobic environment.

<div style="display: flex; align-items: center;"> <div style="writing-mode: vertical-rl; transform: rotate(180deg);">Mass Balance</div> <div style="margin-left: 10px;"> <div style="border-bottom: 1px solid black; width: 100px; height: 2px; margin-bottom: 5px;"></div> <div style="display: flex; align-items: center;"> <div style="width: 10px; height: 10px; border: 1px solid black; margin-right: 5px;"></div> <div>Continuity</div> </div> </div> </div>		Component →	i	1	2	3	Process rate, $\rho_j$ [ML <sup>-3</sup> T <sup>-1</sup> ]
		j	Process ↓	$X_B$	$S_B$	$S_0$	
	1	Growth		1	$-\frac{1}{Y}$	$-\frac{1-Y}{Y}$	$\frac{\hat{\mu}S}{K_s + S_s} X_B$
	2	Decay		-1		-1	$bX_B$
	Observed Conversion Rates [ML <sup>-3</sup> T <sup>-1</sup> ]			$r_i = \sum_j r_{ij} = \sum_j v_{ij}\rho_j$			Kinetic Parameters:
	Stoichiometric Parameters:						Maximum specific growth rate: $\hat{\mu}$
	True Growth Yield: $Y$			Biomass [M(COD)L <sup>-3</sup> ]	Substrate [M(COD)L <sup>-3</sup> ]	Oxygen (negative COD) [M(-COD)L <sup>-3</sup> ]	Half-velocity constant: $K_s$
							Specific decay rate: $b$

The first step in setting up the matrix is to identify the components of relevance in the model. In this scenario these are biomass, substrate, and dissolved oxygen, which are listed across the top of Table 1.1 by symbol and across the bottom by name and units. To conform with IAWPRC nomenclature (Grau *et al.* 1982), insoluble constituents are given the symbol  $X$  and soluble components  $S$ . Subscripts are used to specify individual components: B for biomass, S for substrate, and O for oxygen. The index  $i$  is assigned to each component. In this case,  $i$  ranges from 1 to 3 for the three compounds in this simple model.

The second step in developing the matrix is to identify the biological processes occurring in the system, i.e. the conversions or transformations that affect the components listed. Only two processes are included in this example: aerobic growth of biomass and its loss by decay. These processes are listed in the leftmost column of the matrix. The index  $j$  is assigned to each process: in this case,  $j = 1$  or 2.

The kinetic expressions or rate equations for each process are recorded in the rightmost column of the matrix in the appropriate row. Process rates are denoted by  $\rho_j$  where  $j$  corresponds to the process as numbered in the leftmost column. If we were to use the simple Monod–Herbert (Herbert 1958) model for this situation, the rate expressions would be those in Table 1.1. The Monod equation,  $\rho_1$ , says that growth of biomass is proportional to biomass concentration in a first-order manner and to substrate concentration in a mixed-order manner. The Herbert expression,  $\rho_2$ , states that biomass decay is first-order with respect to biomass concentration. The kinetic parameters used in the rate expressions are defined in the lower right corner of the table.

The elements within the matrix comprise the stoichiometric coefficients,  $v_{ij}$ , which set out the mass relationships between the components in the individual processes. For example, growth of biomass (+1) occurs at the expense of soluble substrate ( $-1/Y$ ); oxygen is utilised in the metabolic process [ $-(1-Y)/Y$ ]. The coefficients,  $v_{ij}$ , are greatly simplified by working in consistent units. In this case, all organic constituents have been expressed as equivalent amounts of chemical oxygen demand (COD); likewise, oxygen is expressed as negative

oxygen demand. The sign convention used in the matrix is negative for consumption and positive for production. All stoichiometric parameters are defined in the lower left corner of the table.

### 1.5.2 Use in mass balances

Within a system, the concentration of a single component may be affected by a number of different processes. An important benefit of the matrix representation is that it allows rapid and easy recognition of the fate of each component, which aids in the preparation of mass balance equations. This may be seen by moving down the column representing a component, which is why the arrow marked “Mass Balance” is placed at the left-hand side. The basic equation for a mass balance within any defined system boundary is:

$$\text{Input} - \text{Output} + \text{Reaction} = \text{Accumulation} \quad (1.2)$$

The input and output terms are transport terms and depend upon the physical characteristics of the system being modelled. The system reaction term,  $r_i$ , is obtained by summing the products of the stoichiometric coefficients  $v_{ij}$  and the process rate expression  $\rho_j$  for the component  $i$  being considered in the mass balance:

$$r_i = \sum_j v_{ij} \rho_j \quad (1.3)$$

For example, the rate of reaction,  $r$ , for biomass,  $X_B$ , at a point in the system would be:

$$r_{X_B} = \frac{\mu S_s}{K_s + S_s} X_B - b X_B \quad (1.4)$$

for soluble substrate,  $S_s$ , it would be:

$$r_{S_s} = -\frac{1}{Y} \frac{\mu S_s}{K_s + S_s} X_B \quad (1.5)$$

for dissolved oxygen,  $S_O$ , it would be:

$$r_{S_O} = -\left(\frac{1-Y}{Y}\right) \frac{\mu S_s}{K_s + S_s} X_B - b X_B \quad (1.6)$$

To create the mass balance for each component within a given system boundary (e.g. a completely mixed reactor), the conversion rate would be combined with the appropriate advective (flow) terms for the particular system. These terms have not been shown here because the purpose of the example is to demonstrate how the matrix is used to define the

fundamental reactions regardless of the system configuration. It should be emphasised, however, that the modelling of a particular physical system requires definition of the system boundary with the associated advective terms.

### 1.5.3 Mass conservation check

Another benefit of the matrix is that mass conservation can be checked by moving across the matrix; the sum of the stoichiometric coefficients multiplied by the mass fraction coefficients characterising the composition of the substances must be zero, if all substances affected by the process are considered in the matrix. This can be demonstrated by considering the decay process. Recalling that oxygen is negative COD so that its coefficient must be multiplied by  $-1$ , all COD lost from the biomass because of decay must be balanced by oxygen utilisation. Similarly, for the growth process, the substrate COD lost from solution due to growth minus the amount converted into new cells must equal the oxygen used for cell synthesis.

Application of the mass conservation concept disqualifies the use of the traditional measure of organic matter in streams, BOD, in the process descriptions for RWQM1 since mass balances are not possible with BOD. The BOD test measures part of the material present, and measures varying parts depending upon the history of the organic material. The more oxidation the organic material has undergone, the smaller will the fraction be that is measured as BOD. For raw wastewater, typically 50% of the organic material is measured, while in biologically treated wastewater only 10–20% is measured. After degradation of part of the organic material in wastewater during its transport in a river, less than 5% of the organic material may be measured with the BOD test.

### 1.5.4 Terminology

The Petersen matrix approach employs as terminology “components” to represent the chemical and biological species in the model and “processes” to represent the conversions or transformations that affect the components. In the context of environmental water quality modelling, we must add several additional terms. The term “compartment” is used to denote the conceptual subdivision of the system into different biochemical or physical environments. For example, it is typical to include separate compartments for the water column and the sediment. Appendix 1 presents an ecologically-based definition of the river system as a continuum of various zones and the compartments that define those zones.

Yet another term can arise as part of the process of solving the model equations. Formulation of a finite-element, finite-difference, or otherwise spatially segmented model requires that the physical space represented in the model be subdivided. This creates spatial segments, which can go by a variety of names including spatial elements, finite-difference elements or grids, finite elements, and boxes. Although there is necessarily some relationship between model compartments and spatial segments, the latter arise from the method of solving the equations, whereas compartments are a more fundamental characteristic of the model.

The term “state variable” indicates the model variables that must be solved for. The number of state variables is equal to the number of compartments multiplied by the number of components. Typical state variables are the concentrations of phosphorus in the water phase in the water column compartment, the interstitial water phase in the sediment compartment, and the adsorbed phase within the sediment compartment.

In addition, the model includes a number of “parameters.” These are the various rate constants, proportionality coefficients, temperature-dependency coefficients, and other



coefficients and constants that must be defined in the transport and process equations. Table 1.1, for example, defines several process and stoichiometric parameters in the model of heterotrophic bacterial growth. Model parameters are distinct from water quality parameters, in which case the term is used to represent some measurement of the state of the water quality in the environment. For example, the concentration of dissolved oxygen is a water quality parameter.

## 1.6 ABOUT THE PROCESS OF MODEL DEVELOPMENT

We believe that achieving all of the objectives outlined above will require about a decade-long process of model development that includes such difficult tasks as improving the description of sediment processes. Our primary goal is only to launch this process, to define the framework, and to provide a first model version<sup>2</sup> that we hope can be extended and further developed by a broad range of professionals dealing with water quality issues.

Some readers of this report will seek a model “code”, that is, a computer program for application of the model. As with ASM1, our intention was not to create a code *per se*, but rather a conceptual model framework than can be implemented in a variety of codes. We have implemented the model in AQUASIM (Reichert 1994, 1995), a proprietary code available from EAWAG (<http://www.aquasim.eawag.ch>), and Meirlaen *et al.* (2001a,b) have implemented the model in the WEST modelling and simulation software (Vangheluwe *et al.*, 1996, 1998, <http://www.hemmiswest.com/>). Meirlaen *et al.*'s application took particular advantage of RWQM1's capability to integrate sewer and ASM-like models to simulate integrated real-time control of an urban wastewater system. Moreover, we encourage potential program users to create model versions in a variety of frameworks such as the US EPA WASP program (Ambrose *et al.* 1988), Matlab (<http://www.mathworks.com/products/matlab/>), Microsoft® Excel (<http://www.microsoft.com/products/default.asp>), and user-developed codes.

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<sup>2</sup> In the course of our work the conversion model obviously went through modifications. In relation to this, we note that the case studies in Chapter 5 demonstrate results obtained by the application of the “first” model version (Reichert *et al.* 2001a), while Chapter 3 presents a somewhat extended “second” version we felt to be the most relevant as we proceeded with our effort. Despite the creation of two versions of the model, we do not make a distinction such as RWQM1 and RWQM2 since the difference is not significant to the case studies because the “second”, extended version still contains the “first” version as a special case.